Poster Presentation

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Acyl-transfer reactions in molecular crystals: reactivity correlation with crystal structure

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Reactions in molecular crystals apart from being environmentally green, offer high product selectivity and specificity due to constrained environment of the crystal lattice. The reactivity of molecules is essentially controlled due to the proximity of the reactive groups and their inability to freely move in the crystal. Hence, these reactions also delineation of mechanistic pathways of the reaction. We are interested in acyl transfer reactions in molecular crystals.[1-3] We had shown that the relative geometry of electrophile and nucleophile, non-covalent interactions which supplements their 'pre-organization' as well as the discrete assembly of reactive molecules that allow a domino type of reaction are essential for efficient acyl transfer between molecules in crystals. Based on these parameters we could even identify potential cocrystal by survey of the Cambridge Structural Database (CSD) that showed efficient acyl transfer reactivity in crystalline state. We have recently extended these studies to intramolecular acyl transfer reactions. Correlation between the crystal structure and the specific solid state reactivity of the molecular solids has wider implications for the development of solid-state organic reactions as a tool for organic synthesis. These aspects will be discussed.

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